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Higher-order $\hbar$ corrections in the semiclassical quantization of chaotic billiards

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Abstract. In the periodic orbit quantization of physical systems, usually only the leading-order $\hbar$ contribution to the density of states is considered. Therefore, by construction, the eigenvalues following from semiclassical trace formulae generally agree with the exact quantum ones only to lowest order of $\hbar$. In different theoretical work the trace formulae have been extended to higher orders of $\hbar$. The problem remains, however, how to actually calculate eigenvalues from the extended trace formulae since, even with $\hbar$ corrections included, the periodic orbit sums still do not converge in the physical domain. For *lowest-order* semiclassical trace formulae the convergence problem can be elegantly, and universally, circumvented by application of the technique of harmonic inversion. In this paper we show how, for general scaling chaotic systems, also *higher-order* $\hbar$ corrections to the Gutzwiller formula can be included in the harmonic inversion scheme, and demonstrate that corrected semiclassical eigenvalues can be calculated despite the convergence problem. The method is applied to the open three-disk scattering system, as a prototype of a chaotic system.

PACS. 03.65.Sq Semiclassical theories and applications

1 Introduction

The relation between the eigenvalue spectrum of a quantum system and the periodic orbits of the corresponding classical system is a question of fundamental importance for both integrable and chaotic dynamical systems. The well-established Gutzwiller trace formula [1,2,3] for classically chaotic systems and its analogue for integrable systems, the Berry-Tabor formula [4,5], provide the semiclassical density of states in terms of a sum over all periodic orbits of the system. However, each trace formula is only the leading-order term of an expansion of the exact density of states in powers of $\hbar$, and therefore in general the resulting semiclassical eigenvalues are only approximations to the exact quantum ones. In recent years, two basic methods have been developed for determining higher-order $\hbar$ corrections to the Gutzwiller trace formula in terms of periodic orbit contributions [6,7,8,9,10,11]. Unfortunately, even with $\hbar$ corrections included, the trace formulae usually suffer from being divergent in the region where the physical eigenvalues or resonances are located. For specific systems, higher-order $\hbar$ corrections to the semiclassical eigenvalues have explicitly been calculated by cycle expansion techniques [6,9,10]. However, this method is applicable only to systems with special features, namely to hyperbolic systems with a known complete symbolic dynamics.

Recently, it has been demonstrated how the convergence problems of the semiclassical trace formulae can be circumvented by the application of harmonic inversion techniques [12,13,14]. The harmonic inversion method is capable of extracting semiclassical eigenvalues from a finite set of periodic orbits with very high precision and resolution. In contrast to other semiclassical methods, harmonic inversion does not require any special properties of the system, and can therefore be applied to a wide range of physical systems. In Refs. [14,15,16] a general procedure has been developed for including higher-order $\hbar$ corrections to the trace formulae in the harmonic inversion scheme. So far, this method has only been tested for an integrable system, viz. the circle billiard. The general procedure, however, does not depend on the type of the underlying classical dynamics, and is applicable also to chaotic systems. In this paper, we demonstrate how the method works for chaotic systems, and apply it to the open three-disk scatterer, which has become a standard example for the semiclassical quantization of chaotic systems [13,14,17,18,19,20,21].

The harmonic inversion method is used in two directions: First, we carry out a harmonic analysis of the spectrum of the differences between the exact (complex) quantum eigenvalues and the semiclassical resonances of the three-disk system. We show how this enables one to determine, for each orbit, the first-order $\hbar$ correction term (and, in principle, all higher-order correction terms) to the Gutzwiller formula. We confirm our results by comparing with the values

calculated by a specialization of an analytical approach developed by Vattay and Rosenqvist [8,9] for two-dimensional billiards [10]. Second, we take the analytical correction terms to the Gutzwiller formula and compute, using the classical periodic orbit data and harmonic inversion, the first-order $\hbar$ corrections to the semiclassical resonances of the three-disk system. Thus we illustrate that corrected semiclassical eigenvalues can be calculated by harmonic inversion despite the convergence problems of the trace formulae. We compare the zeroth and first-order approximations to the resonances with the exact quantum eigenvalues, and can quantitatively assess the increase in accuracy produced by including the next-order corrections.

2 Higher-order $\hbar$ corrections to Gutzwiller's trace formula

Gutzwiller's trace formula for chaotic systems gives a semiclassical approximation to the response function (i.e., the trace of the Green's function) of a quantum system in terms of the periodic orbits of the corresponding classical system. The semiclassical response function consists of a smooth background, and an oscillating part $g(E) = \bar{g}(E) + g^{\rm osc}(E)$, where the oscillating part is given by [3,22]

$$g^{\rm osc}(E) = -{\rm i} \sum_{\rm po} \frac{T_{\rm po}}{r|\det(M_{\rm po} - \mathbf{1})|^{1/2}} \exp\left[{\rm i}\left(\frac{S_{\rm po}}{\hbar} - \mu_{\rm po}\frac{\pi}{2}\right)\right] . \tag{1}$$

The sum in (1) runs over all periodic orbits (po) of the system, including multiple traversals. Here, $T_{\rm po}$ and $S_{\rm po}$ are the period and the action of the orbit, $M_{\rm po}$ and $\mu_{\rm po}$ denote the monodromy matrix and the Maslov index, and the repetition number r counts the traversals of the underlying primitive orbit ("primitive" means that there is no sub-period). The semiclassical density of states $\rho(E)$ is related to the response function via

$$\rho(E) = -\frac{1}{\pi} \, {\rm Im}\, g(E) . \tag{2}$$

In general, the semiclassical eigenvalues or resonances obtained from the Gutzwiller formula agree with the exact quantum ones only in leading order of $\hbar$. To improve the accuracy of the semiclassical eigenvalues, higher-order $\hbar$ correction terms to the Gutzwiller formula have to be included. Two different methods for the calculation of such higher-order $\hbar$ terms have been derived for chaotic systems, one by Gaspard and Alonso [6,7], and the other by Vattay and Rosenqvist [8,9,10]. The latter method has been specialized to two-dimensional chaotic billiards in Ref. [10]. An extension of the method of Gaspard and Alonso has recently been published in Ref. [11]. We will adopt the method of Vattay and Rosenqvist to compute the first-order $\hbar$ corrections to the semiclassical resonances of the open three-disk scatterer.

Vattay and Rosenqvist give a quantum generalization of the Gutzwiller formula, which is of the form

$$g(E) = \bar{g}(E) + \frac{1}{{\rm i}\hbar} \sum_p \sum_l \left(T_p(E) - {\rm i}\hbar \frac{{\rm d}\ln R_p^l(E)}{{\rm d}E} \right) \sum_{r=1}^{\infty} \left(R_p^l(E)\right)^r \exp\left(\frac{\rm i}{\hbar} r S_p(E)\right). \tag{3}$$

The first sum runs over all *primitive* periodic orbits; T_p and S_p are the traversal time and the action of the periodic orbit, respectively. The sum over r corresponds to multiple traversals of the primitive orbit. The quantities R_p^l are associated with the local eigenspectra determined by the local Schrödinger equation in the neighbourhood of the periodic orbits. An expansion of the quantities R_p^l in powers of $\hbar$,

$$\begin{aligned} R^l(E) &= \exp\left\{ \sum_{m=0}^{\infty} \left(\frac{{\rm i}\hbar}{2}\right)^m C_l^{(m)} \right\} \\ &\approx \exp\left(C_l^{(0)}\right) \left(1 + \frac{{\rm i}\hbar}{2} C_l^{(1)} + \dots\right) , \end{aligned} \tag{4}$$

yields the $\hbar$ expansion of the generalized trace formula (3). For two-dimensional hyperbolic systems, the zeroth-order terms are given by

$$\exp\left(C_l^{(0)}\right) = \frac{{\rm e}^{{\rm i}\mu_p \pi/2}}{|\lambda_p|^{1/2} \lambda_p^l} , \tag{5}$$

where μ_p and λ_p are the Maslov index and the expanding stability eigenvalue (i.e., the stability eigenvalue with an absolute value larger than one) of the orbit, respectively. By summation over l, the Gutzwiller trace formula is regained

as zeroth-order approximation to Eq. (3). If the zeroth-order terms do not depend on the energy, as is the case for billiard systems, the first-order correction to the Gutzwiller formula can be written as

$$g_1(E) = \frac{1}{\mathrm{i}\hbar} \sum_{\mathrm{po}} \sum_{l} \frac{T_{\mathrm{po}}(E)}{r} \exp\left(C_l^{(0)}\right) \frac{\mathrm{i}\hbar}{2} C_l^{(1)} \exp\left(\frac{\mathrm{i}}{\hbar} S_{\mathrm{po}}(E)\right) , \tag{6}$$

where the first sum in Eq. (6) now runs over *all* periodic orbits, including multiple traversals, and r is the repetition number with respect to the underlying primitive orbit.

An explicit recipe for the calculation of the correction terms $C_l^{(1)}$ for two-dimensional chaotic billiards was given in Ref. [10]. The correction terms must in general be calculated numerically from the periodic orbit data. A numerical code which determines the first-order corrections for two-dimensional chaotic billiards can also be found in Ref. [10]. We have used that code to compute the correction terms $C_l^{(1)}$ for the three-disk system for a comparison with the correction terms calculated by harmonic inversion.

3 The open three-disk scatterer

As a model system for the calculation of higher-order $\hbar$ corrections to the Gutzwiller formula by harmonic inversion, we consider the open three-disk system, which consists of three equally spaced hard disks of unit radius. This system, in particular the case of the relatively large disk separation $d = 6$, has served as an archetype for the application of semiclassical quantization techniques in many investigations in recent years [13,14,18,19,20,21]. We will consider the case $d = 6$, as well as the small separation $d = 2.5$. In our calculations, we make use of the symmetry reduction of the three-disk system introduced in Refs. [18,23] and concentrate on states of the A_1 subspace.

As for all billiard systems, the shape of the periodic orbits in the three-disk system is independent of the wave number $k = \sqrt{2mE}/\hbar$, and the action scales as

$$S/\hbar = ks, \tag{7}$$

where the scaled action s is equal to the physical length of the orbit. We consider the density of states as a function of the wave number

$$\rho(k) = -\frac{1}{\pi} \operatorname{Im} g(k) , \tag{8}$$

with a scaled response function $g(k)$. Since the wave number k is proportional to $\hbar^{-1}$, it can be considered as an effective Planck constant,

$$k = \hbar_{\mathrm{eff}}^{-1} . \tag{9}$$

The $\hbar$ expansion of the exact quantum response function can therefore be written as a power series in k^{-1}:

$$g(k) = \bar{g}(k) + g^{\mathrm{osc}}(k) \tag{10}$$

with

$$g^{\mathrm{osc}}(k) = \sum_{n=0}^{\infty} g_n(k) = \sum_{n=0}^{\infty} \frac{1}{k^n} \sum_{\mathrm{po}} \mathcal{A}_{\mathrm{po}}^{(n)} \mathrm{e}^{\mathrm{i} s_{\mathrm{po}} k}. \tag{11}$$

The second sum runs over all periodic orbits including multiple traversals. The zeroth-order amplitudes $\mathcal{A}_{\mathrm{po}}^{(0)}$ correspond to the Gutzwiller formula, whereas for $n > 0$, the amplitudes $\mathcal{A}_{\mathrm{po}}^{(n)}$ give the n^{th}-order corrections $g_n(k)$ to the response function.

Applying the Gutzwiller trace formula to the (symmetry reduced) three-disk system yields for the zeroth-order amplitudes in Eq. (11) (A_1 subspace)

$$\begin{aligned} \mathcal{A}_{\mathrm{po}}^{(0)} &= -\mathrm{i} \sum_{\mathrm{po}} \frac{s_{\mathrm{po}} \, \mathrm{e}^{-\mathrm{i}\frac{\pi}{2}\mu_{\mathrm{po}}}}{r |\det(M_{\mathrm{po}} - 1)|^{1/2}} \\ &= -\mathrm{i} \sum_{\mathrm{po}} (-1)^{l_s} \frac{s_{\mathrm{po}}}{r|(\lambda_{\mathrm{po}} - 1)(\frac{1}{\lambda_{\mathrm{po}}} - 1)|^{1/2}} , \end{aligned} \tag{12}$$

where M_{po} is the monodromy matrix of the orbit, l_s is the symbol length, s_{po} the scaled action, and λ_{po} the expanding stability eigenvalue of the orbit. The Maslov index μ_{po} for this system is given by $2l_s$. The quantity r designates the repetition number with respect to the corresponding primitive orbit. The first-order amplitudes of the $\hbar$ expansion (11) following from Eq. (6) read

$$\mathcal{A}_{\mathrm{po}}^{(1)} = \frac{s_{\mathrm{po}}}{r} \sum_{l} \frac{(-1)^{l_s}}{|\lambda_{\mathrm{po}}|^{1/2} \lambda_{\mathrm{po}}^{l}} \frac{C_l^{(1)}}{2\hbar k} . \tag{13}$$

Since the terms $C_l^{(1)}$ are proportional to the momentum $\hbar k$, as was shown in Ref. [10], the amplitudes are independent of the scaling parameter k. The correction terms $C_l^{(1)}$ have to be determined numerically. We use the code developed by Rosenqvist and Vattay [10,24]. The code requires the flight times between the bounces and the reflection angles as an input. These parameters have to be calculated numerically for each periodic orbit. As the contributions to the amplitude (13) for different l are proportional to $|\lambda_{\rm po}|^{-l-\frac{1}{2}}$, the sum over l converges fast if the absolute value of the stability eigenvalue $\lambda_{\rm po}$ is large. For most orbits, the leading term $l = 0$ turns out to be already sufficient. It is only for the very shortest orbits that terms of higher order in l have to be included to ensure convergence of the sum to within, say, 3 significant digits.

4 Harmonic analysis of the quantum spectrum

4.1 Theory

In Refs. [14,16] it was demonstrated that the amplitudes $\mathcal{A}_{\rm po}^{(n)}$ of the $\hbar$ expansion (11) can be obtained by a harmonic inversion analysis of the exact quantum spectrum. The general procedures do not depend on any special properties of the system and can be applied to both integrable and chaotic systems. In Ref. [16], they were tested for the circle billiard, as an example of an integrable system. We will now use the same procedures for the open three-disk system, as a representative of a chaotic system.

We start by briefly recapitulating the main ideas of the procedures developed in Refs. [14,16]. The exact quantum mechanical response function, in terms of the wave number k, can be written as

$$g^{\rm qm}(k) = \sum_j \frac{m_j}{k - k_j + {\rm i}0} \,, \tag{14}$$

where the k_j are the exact eigenvalues or resonances of k, and m_j are their multiplicities. Eq. (11) gives the $\hbar$ expansion of (14) in terms of periodic orbit contributions. The first-order amplitudes $\mathcal{A}_{\rm po}^{(0)}$ of the expansion (11) can be determined by adjusting the exact response function (14) to the form of the semiclassical approximation

$$g^{\rm osc}(k) \approx \sum_{\rm po} \mathcal{A}_{\rm po}^{(0)} {\rm e}^{{\rm i}ks_{\rm po}} \tag{15}$$

by harmonic inversion [25]. Note that for chaotic billiards the leading-order amplitudes $\mathcal{A}_{\rm po}^{(0)}$ as well as the higher-order amplitudes $\mathcal{A}_{\rm po}^{(n)}$ are independent of the wave number k. In a direct harmonic analysis of the quantum spectrum only the zeroth-order term of the expansion (11) fulfills the ansatz for the harmonic inversion procedure. The higher-order terms act as a kind of weak noise which is separated from the zeroth-order "signal" by the harmonic inversion procedure. The direct harmonic analysis of the quantum signal will therefore yield exactly the lowest-order amplitudes $\mathcal{A}_{\rm po}^{(0)}$.

The $n^{\rm th}$-order amplitudes $\mathcal{A}_{\rm po}^{(n)}$ can be determined if the exact eigenvalues k_j and their $(n-1)^{\rm st}$-order approximations $k_{j,n-1}$ are given. The $(n-1)^{\rm st}$-order approximation to the response function can be written in the form (14), with k_j replaced with the approximation $k_{j,n-1}$. One can then calculate the difference between the exact quantum mechanical and the $(n-1)^{\rm st}$-order response function and compare it with the expression resulting from the expansion (11),

$$g^{\rm qm}(k) - \sum_{m=0}^{n-1} g_m(k) = \sum_{m=n}^{\infty} g_m(k) = \sum_{m=n}^{\infty} \frac{1}{k^m} \sum_{\rm po} \mathcal{A}_{\rm po}^{(m)} {\rm e}^{{\rm i}s_{\rm po}k} . \tag{16}$$

The leading-order terms in (16) are $\sim k^{-n}$, i.e., multiplication by k^n yields

$$k^n \left[g^{\rm qm}(k) - \sum_{m=0}^{n-1} g_m(k) \right] = \sum_{\rm po} \mathcal{A}_{\rm po}^{(n)} {\rm e}^{{\rm i}s_{\rm po}k} + \mathcal{O}\left(\frac{1}{k}\right) \,. \tag{17}$$

The right-hand side of (17) now has assumed a form which is again suited to the harmonic inversion procedure. More precisely, the harmonic inversion of the weighted difference spectrum (17) will yield the periods $s_{\rm po}$ and the $n^{\rm th}$-order amplitudes $\mathcal{A}_{\rm po}^{(n)}$ of the $\hbar$ expansion (11).

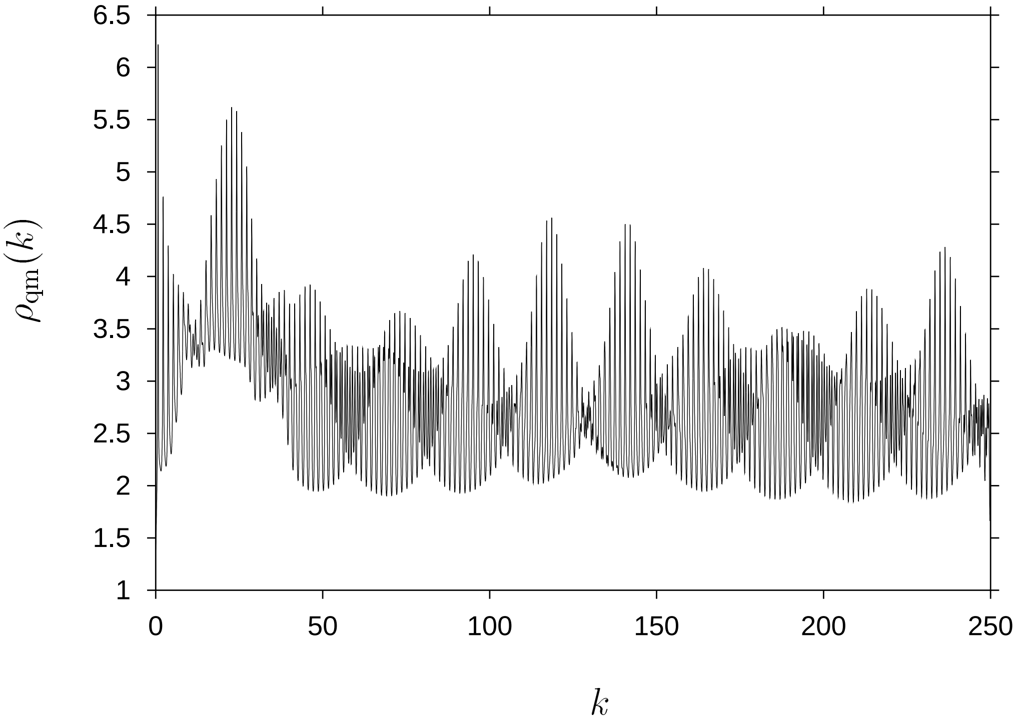

Fig. 1. Quantum mechanical density of states $\rho(k) = (-1/\pi)\,\mathrm{Im}\,g(k)$ of the three-disk system with disk separation $d = 6$ (A_1 subspace) as a function of real values of the wave number k. Only resonances of the four leading bands have been included. [Data courtesy of A. Wirzba.]

4.2 Application to the three-disk scattering system

We now apply the procedure to the three-disk system with disk separation $d = 6$. As a first step we perform a harmonic analysis of the exact quantum spectrum to obtain the leading-order ($n = 0$) periodic orbit contributions to the density of states. The exact quantum values for $d = 6$ were taken from Wirzba [21,26,27]. Figure 1 shows the quantum mechanical density of states $\rho(k) = (-1/\pi)\,\mathrm{Im}\,g(k)$ for real values of the wave number k resulting from the four leading bands of the A_1 subspace. Note that this set of resonances is of course not complete as the subleading bands with large negative imaginary part are not included.

The spectrum in Figure 1 served as the signal for the harmonic inversion procedure. The results of the analysis turned out to be more accurate if the lowest part of the signal, determined by the "most quantum" resonances with very small real part, is cut off. We analyzed the spectrum in the range $\mathrm{Re}\,k \in [50, 250]$ to obtain the periodic orbit contributions in two different intervals of the scaled action. The results are presented in Figure 2. The solid lines give the sizes of the imaginary parts of the semiclassical amplitudes $\mathcal{A}_{\mathrm{po}}^{(0)}$ calculated directly from Eq. (12) using the classical periodic orbit data, as a function of the scaled action of the orbits. The crosses show the amplitudes resulting from the harmonic inversion of the quantum spectrum. Note the different scales of the two plots. The results of the harmonic inversion are seen to be in excellent agreement with those from the classical calculations of the amplitudes $\mathcal{A}_{\mathrm{po}}^{(0)}$ entering into Gutzwiller's trace formula, clearly confirming the validity of the latter.

In a second step, we now determine the next-to-leading-order $\hbar$ corrections to the Gutzwiller trace formula for the three-disk system by the harmonic analysis of the difference spectrum between the exact quantum resonances and the semiclassical resonances of the A_1 subspace. The semiclassical resonances for disk separation $d = 6$ had been calculated by Wirzba [21,26,27] from a cycle expansion of the Gutzwiller-Voros zeta function. [Since the Gutzwiller-Voros zeta function is directly related to the Gutzwiller trace formula without further approximations, the semiclassical resonances resulting from both expressions will be the same.] The weighted difference spectrum is shown in Figure 3. Note that due to the limited radius of convergence of the cycle expansion only resonances with $\mathrm{Im}\,k \gtrsim -0.8$ were available and could be included in the signal.

In Figure 4, the crosses designate the results for the first-order amplitudes $\mathcal{A}_{\mathrm{po}}^{(1)}$ obtained from the harmonic inversion of the difference spectrum shown in Fig. 3, which was analyzed in the region $\mathrm{Re}\,k \in [100, 250]$. For comparison, we also determined the first-order amplitudes $\mathcal{A}_{\mathrm{po}}^{(1)}$ for each orbit following the method of Vattay and Rosenqvist described above (see Eq. (13)). These results are represented in Figure 4 by solid lines.

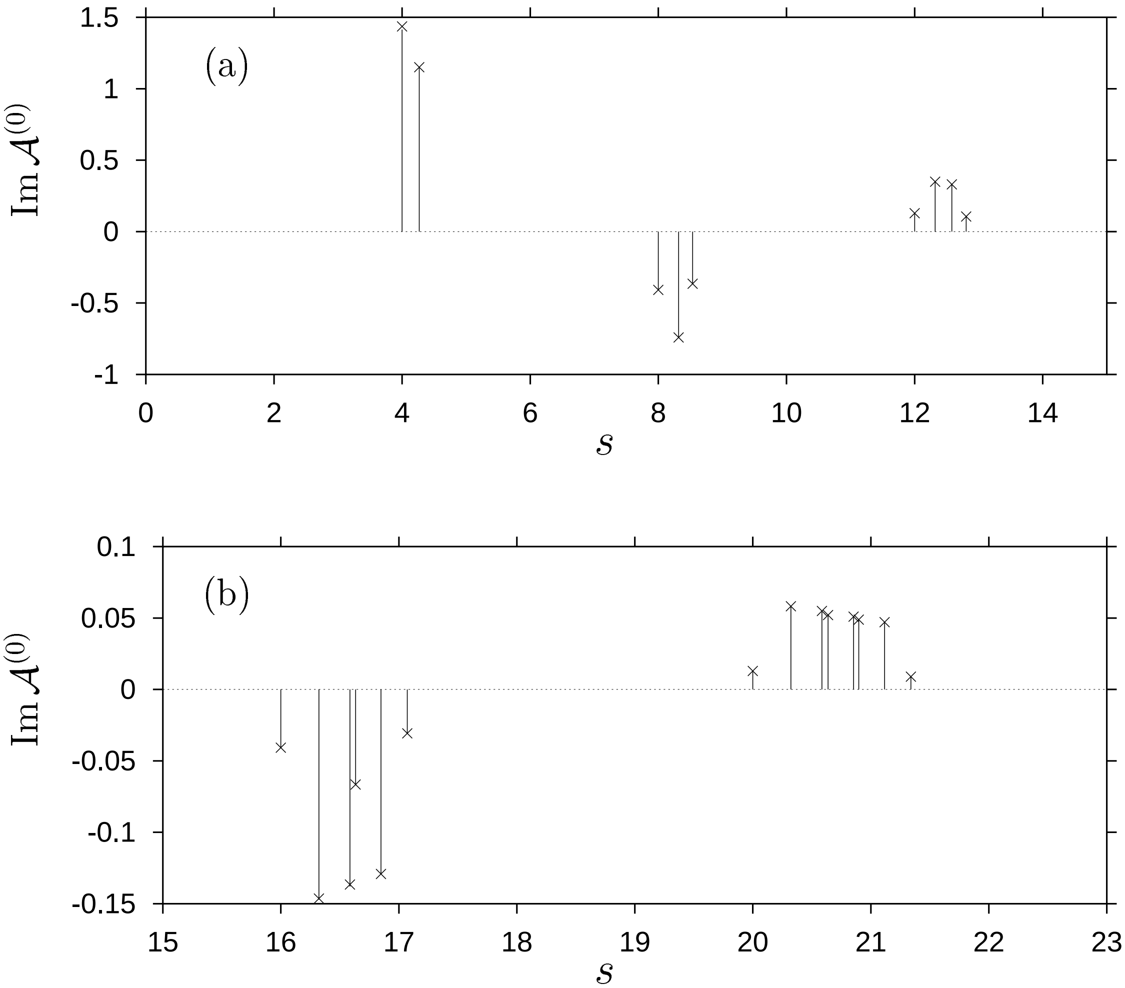

Fig. 2. Imaginary parts of the amplitudes of the leading-order ($n = 0$) periodic orbit contributions to the density of states of the three-disk system with disk separation $d = 6$ as a function of the scaled actions of the symmetry reduced orbits. Solid lines: semiclassical amplitudes $\mathcal{A}_{\rm po}^{(0)}$ versus scaled actions of the symmetry reduced orbits, calculated directly from classical mechanics. Crosses: results from the harmonic inversion of the exact quantum spectrum (A_1 subspace).

For almost all orbits, the harmonic inversion results for $\mathcal{A}_{\rm po}^{(1)}$ are seen to be in perfect agreement with the amplitudes calculated by the method of Refs. [8,9,10]. There is, however, one exception, namely the distinct discrepancy for the orbit with symbolic code ‘1’ (scaled action $s \approx 4.267949$). The deviation is systematic and appears in the same way if the parameters of the harmonic inversion procedure (such as signal length etc.) are varied. This point still needs further clarification. A possible explanation for the discrepancy may lie in the fact that the set of resonances from which the signal was constructed was not complete, since only resonances near the real axis could be included. However, this does not explain why only one orbit is strongly affected. On the other hand, the error might also be due to the theory of Refs. [8,9,10], or its application to the three-disk system. In fact, the ‘1’ orbit is the orbit with the largest contributions from terms of higher order in l to the sum in (13). The contributions from the different l terms and the converged sum over l of the five shortest orbits are given in Table 1. For comparison, the last column of Table 1 shows the corresponding values following from the amplitudes of the harmonic inversion results. The ‘1’ orbit exhibits the largest deviation between the $l = 0$ contribution and the converged sum over l, followed by the ‘0’ orbit. For orbits with a symbol length of 2 or longer, the contributions of higher l terms to the amplitude $\mathcal{A}_{\rm po}^{(1)}$ are already so small (due to the large absolute value of the stability eigenvalue λ) that it is impossible to decide whether or not there is a discrepancy between these terms and the harmonic inversion results. (Note that this is also true for the period doubling of the orbits ‘0’ and ‘1’ in Table 1.) However, the harmonic inversion results for the ‘0’ orbit, which also shows a relatively large contribution from the $l = 1$ term, are in agreement with the theory. Again, it cannot be explained why only the ‘1’ orbit is affected (although in this case the reasons might lie in the special geometrical properties of the ‘0’ orbit).

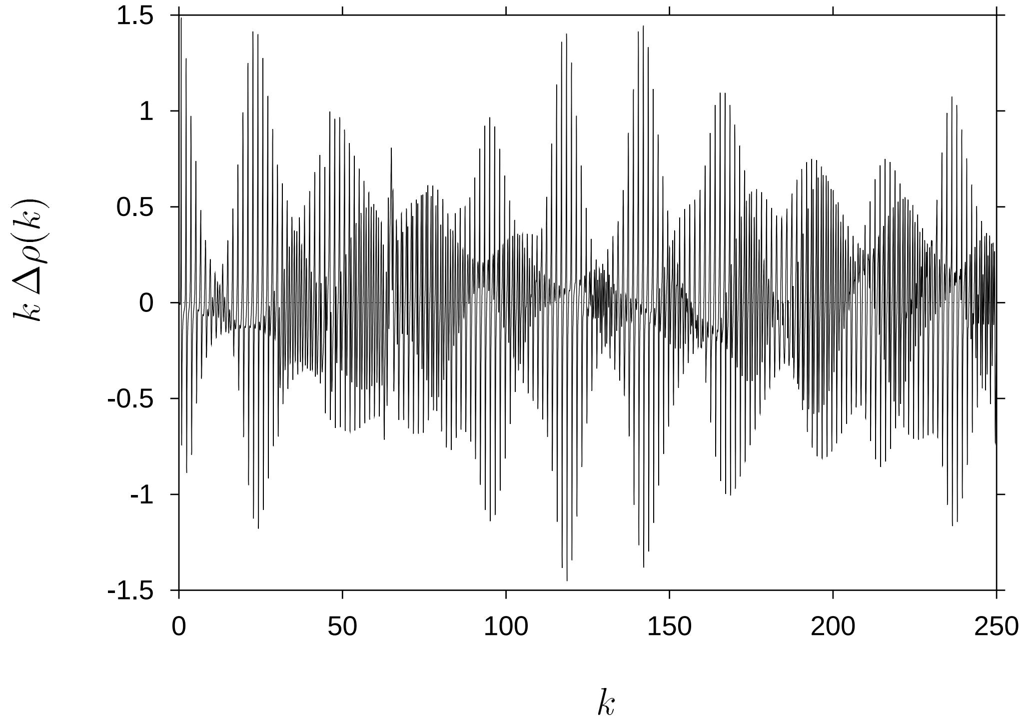

Fig. 3. Three-disk system with disk separation $d = 6$: Weighted difference spectrum $k\,\Delta\rho(k) = k(\rho_{\rm qm}(k) - \rho_{\rm sc}(k))$ between the quantum mechanical and the semiclassical density of states (A_1 subspace) as a function of the wave number k.

Table 1. Correction terms $C_l^{(1)}$ (in units of the momentum $\hbar k$) and their contributions $C_l^{(1)}/\lambda^l$ to the first-order $\hbar$ amplitude (13) for the five shortest periodic orbits of the three-disk system with $d = 6$. The values are compared with the results obtained by harmonic inversion (hi). The orbits are characterized by their symbolic code; their scaled action s and expanding stability eigenvalue λ are also given. Note that the maximum correction to the $l = 0$ contribution occurs for the orbit '1', and is given by the $l = 1$ term.

	l	$C_l^{(1)}$	$\frac{C_l^{(1)}}{\lambda^l}$	$\sum_{l=0}^{\infty} \frac{C_l^{(1)}}{\lambda^l}$	$\left[\sum_{l=0}^{\infty} \frac{C_l^{(1)}}{\lambda^l}\right]_{\rm hi}$
	0	0.625000	0.625000	0.690360	0.6934
'0'	1	1.125000	0.113648		
$s = 4.000000$	2	-2.750000	-0.028064		
$\lambda = 9.898979$	3	-14.750000	-0.015206		
	0	1.124315	1.124315	0.843867	1.055
'1'	1	3.661620	-0.311059		
$s = 4.267949$	2	4.383308	0.031633		
$\lambda = -11.77146$	3	1.162291	-0.000713		
	0	1.250000	1.250000	1.272357	1.259
2×'0'	1	2.250000	0.022962		
$s = 8.000000$	2	-5.500000	-0.000573		
$\lambda = 97.98979$	3	-29.500000	-0.000031		
	0	2.039795	2.039795	1.989582	2.019
'01'	1	6.278740	-0.050596		
$s = 8.316529$	2	5.881196	0.000382		
$\lambda = -124.0948$	3	-4.066328	0.000002		
	0	2.248630	2.248630	2.301937	2.270
2×'1'	1	7.323240	0.052850		
$s = 8.535898$	2	8.766615	0.000457		
$\lambda = 138.5672$	3	2.324582	0.000001		

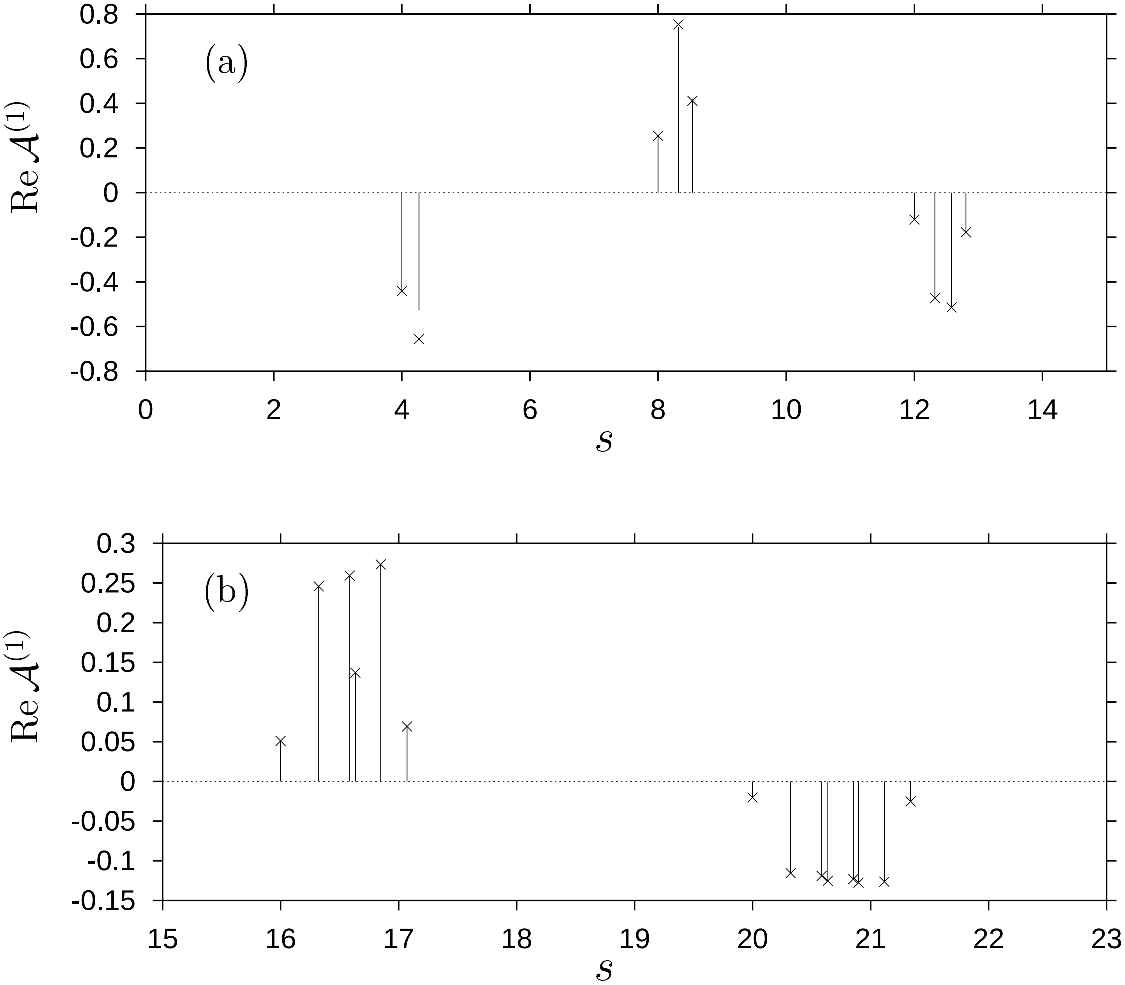

Fig. 4. First-order $\hbar$ corrections to the trace formula of the three-disk system with disk separation $d = 6$ as a function of the scaled actions of the symmetry reduced orbits. Solid lines: first-order amplitudes following from a direct evaluation of Eq. (13). Crosses: results from the harmonic inversion of the difference spectrum between exact quantum resonances and semiclassical cycle expansion values (A_1 subspace).

Concluding our discussion of Figure 4 and Table 1, we notice that the harmonic inversion results indeed confirm the validity of the $l = 0$ approximation to the formula (6) for orbits with large stability eigenvalues. On the other hand, the results demonstrate that the theory of higher-order $\hbar$ corrections to the Gutzwiller formula still contains unanswered questions, and further investigations are necessary.

5 Corrections to the semiclassical eigenvalues

We now turn to the problem of obtaining corrections to the semiclassical eigenvalues of chaotic systems from the $\hbar$ expansion (11) of the periodic orbit sum. A general procedure for including higher-order $\hbar$ corrections in the harmonic inversion scheme was developed in Refs. [14,15,16], where it was applied to the circle billiard as an example of an integrable system. In the following, we briefly recapitulate the main ideas of the procedure and then apply the technique to the open three-disk system.

5.1 Theory

For periodic orbit quantization, usually only the zeroth-order contributions $\mathcal{A}_{\rm po}^{(0)}$ to the expanded response function (11), corresponding to the Gutzwiller formula (or, for integrable systems, the Berry-Tabor formula), are considered. In

the harmonic inversion scheme for semiclassical quantization [12,13,14], semiclassical approximations to the eigenvalues or resonances are determined by adjusting the Fourier transform of the principal periodic orbit sum

$$C_0(s) = \sum_{\rm po} \mathcal{A}_{\rm po}^{(0)} \delta(s - s_{\rm po}) \tag{18}$$

to the functional form of the corresponding exact quantum expression (i.e., the Fourier transform of the exact response function (14))

$$C_{\rm qm}(s) = -{\rm i} \sum_j m_j \, {\rm e}^{-{\rm i}k_j s} \; , \tag{19}$$

with k_j the eigenvalues or resonances and m_j their multiplicities.

Since for $n \geq 1$ the asymptotic expansion (11) of the semiclassical response function suffers from the singularities at $k = 0$, higher-order $\hbar$ terms cannot directly be included in the harmonic inversion scheme. Instead, the correction terms to the semiclassical eigenvalues can be calculated separately, order by order. We assume that the $(n-1)^{\rm st}$-order $\hbar$ approximations $k_{j,n-1}$ to the exact eigenvalues have already been obtained and the $n^{\rm th}$-order approximations $k_{j,n}$ are to be calculated. In terms of these approximations to the eigenvalues, the difference between the two subsequent approximations to the quantum mechanical response function reads

$$\begin{aligned} g_n(k) &= \sum_j \left(\frac{m_j}{k - k_{j,n} + {\rm i}0} - \frac{m_j}{k - k_{j,n-1} + {\rm i}0} \right) \\ &\approx \sum_j \frac{m_j \Delta k_{j,n}}{(k - \bar{k}_{j,n} + {\rm i}0)^2} \; , \end{aligned} \tag{20}$$

with $\bar{k}_{j,n} = \frac{1}{2}(k_{j,n} + k_{j,n-1})$ and $\Delta k_{j,n} = k_{j,n} - k_{j,n-1}$. Integration of (20) and multiplication by k^n yields

$$\mathcal{G}_n(k) = k^n \int g_n(k) {\rm d}k = \sum_j \frac{-m_j k^n \Delta k_{j,n}}{k - \bar{k}_{j,n} + {\rm i}0} \; . \tag{21}$$

The periodic orbit approximation to (21) is obtained from the term $g_n(k)$ in the periodic orbit sum (11) by integration and multiplication by k^n, yielding

$$\mathcal{G}_n(k) = -{\rm i} \sum_{\rm po} \frac{1}{s_{\rm po}} \mathcal{A}_{\rm po}^{(n)} {\rm e}^{{\rm i}ks_{\rm po}} + \mathcal{O}\left(\frac{1}{k}\right) \; . \tag{22}$$

One can now Fourier transform both (21) and (22), and obtains ($n \geq 1$)

$$\begin{aligned} C_n(s) &\equiv \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathcal{G}_n(k) {\rm e}^{-{\rm i}ks} {\rm d}k \\ &= {\rm i} \sum_j m_j (\bar{k}_j)^n \Delta k_{j,n} {\rm e}^{-{\rm i}\bar{k}_j s} \qquad (23) \\ &\overset{\rm h.i.}{=} -{\rm i} \sum_{\rm po} \frac{1}{s_{\rm po}} \mathcal{A}_{\rm po}^{(n)} \delta(s - s_{\rm po}) \; . \qquad (24) \end{aligned}$$

Equations (23) and (24) imply that the $\hbar$ expansion of the semiclassical eigenvalues can be obtained, order by order, by adjusting the periodic orbit signal (24) to the functional form of (23) by harmonic inversion (h.i.). The frequencies $\bar{k}_j$ of the periodic orbit signal (24) are the semiclassical eigenvalues or resonances, averaged over different orders of $\hbar$. Note that the accuracy of these values does not necessarily increase with increasing order n. The corrections $\Delta k_{j,n}$ to the eigenvalues are not obtained from the frequencies, but from the amplitudes, $m_j(\bar{k}_j)^n \Delta k_{j,n}$, of the periodic orbit signal.

5.2 Application to the three-disk scattering system

We have applied the above procedure to the open three-disk scatterer with disk separations $d = 6$ and $d = 2.5$. For both cases, we first calculated the zeroth-order $\hbar$ approximations to the resonances and then determined the first-order $\hbar$ corrections to the semiclassical results following the scheme outlined above.

For disk separation $d = 6$, we used the periodic orbits up to length $s_{\max} = 56$ to calculate the resonances in the region $0 \le \mathrm{Re}\,k \le 250$. In the first-order amplitudes (13), only the leading-order term $l = 0$ of the sum was included. (The terms with $l \ge 1$ contribute significantly only to the '1' orbit and thus basically do not effect the semiclassical resonances.) The results for the first-order corrections Δk_1 were added to the semiclassical results to obtain the first-order approximations k_1 to the resonances. Table 2 shows part of the results in the regions $\mathrm{Re}\,k \in [0, 12]$ and $\mathrm{Re}\,k \in [150, 155]$ with $\mathrm{Im}\,k \ge -0.5$. For comparison, the exact quantum resonances k_{ex} from Refs. [21,26,27] are also given. We note that the semiclassical resonances k_0 obtained by harmonic inversion agree with the semiclassical cycle expansion values from Refs. [21,26,27] to all digits given. Figure 5 compares the semiclassical errors of the zeroth-order (crosses) and first-order (squares) approximations as a function of the real part of the resonances. The deviations of the real and imaginary parts from the exact quantum values are shown separately. Only resonances with an imaginary part $\mathrm{Im}\,k \ge -0.5$ were included in the plot.

The results presented in Figure 5 show that by including the first-order corrections a significant improvement in the accuracy of the real parts of the resonances is achieved. This is evident from Figure 5 in spite of the fact that a one-to-one correspondence between the zeroth and first-order values plotted is difficult to establish with the naked eye. For most resonances, the real part of the first-order approximation lies between two and five orders of magnitude closer to the exact quantum values than the zeroth-order approximation. Only for the "most quantum" resonances, with very low real parts, the improvement is rather small. The reason for this lies in the nature of the semiclassical approximation as an approximation itself: in order to improve these values, second or higher-order terms of the $\hbar$ expansion must be considered.

The accuracy of the imaginary parts of the semiclassical resonances is less significantly increased by the first-order corrections than that of the real parts. For some resonances, the zeroth-order approximation lies even closer to the exact quantum values than the first-order approximation. This was also observed in Refs. [6,10], where the first-order $\hbar$ corrections to the resonances was calculated using the cycle expansion technique. As discussed in [6,10], the first-order corrections to the periodic orbit sum mainly improve the real part of the resonances, while the imaginary part can be expected to be improved by second-order $\hbar$ corrections.

A similar behaviour can be found for disk separation $d = 2.5$. Here, we calculated the semiclassical resonances and their first-order $\hbar$ corrections in the range $0 \le \mathrm{Re}\,k \le 90$ and $-0.82 \le \mathrm{Im}\,k \le 0$ from the periodic orbits up to length $s_{\max} = 12$. In the first-order amplitudes (13), again only the $l = 0$ term was included. Table 3 compares part of the results for the first-order approximations to the resonances with the zeroth-order approximations and the exact quantum values. The zeroth order resonances k_0 obtained by harmonic inversion agree with the cycle expansion values calculated by Wirzba [21,26,27] (not shown) to at least four significant digits.

Again, we determined the semiclassical error of the first-order approximations to the resonances in comparison to that of the zeroth-order approximation. The results are presented in Figure 6. The general behaviour of the values is similar to that in the case $d = 6$ discussed above, although the improvement of the accuracy achieved by the first-order corrections is not as spectacular as for $d = 6$. The reason for this may partly lie in the error induced by the harmonic inversion method, which for $d = 2.5$ is larger already in the zeroth-order approximation than for $d = 6$. The results could in principle be improved by extending the signal to longer orbits. On the other hand, in the part of the spectrum considered, second and higher-order $\hbar$ corrections may be more important than in the case $d = 6$. However, it is evident from Figure 6 that, apart from the resonances with very small real parts, the semiclassical error of the real parts of the resonances could still be reduced, even for the small disk separation of $d = 2.5$, by the first-order $\hbar$ corrections by one or two orders of magnitude.

6 Conclusions

In this paper we have demonstrated the power of the harmonic inversion technique in explicitly determining higher-order $\hbar$ corrections to the Gutzwiller trace formula and to the semiclassical eigenvalues of a completely chaotic system, namely the three-disk scattering system. The method has been used in two directions: (1) for the harmonic analysis of the exact quantum spectrum, (2) for the direct calculation of higher-order corrections to the semiclassical eigenvalues from classical periodic orbit data.

The harmonic analysis of the exact quantum spectrum of the three-disk system with the "standard" literature disk separation of $d = 6$ first yielded the zeroth-order semiclassical amplitudes of the periodic orbit sum (i.e., the amplitudes entering the Gutzwiller formula), which were found to be in perfect agreement with the Gutzwiller amplitudes calculated directly from classical periodic orbit data. Next, from the exact quantum resonances and their zeroth order approximations, we were able to compute the first-order amplitudes applying harmonic inversion to Eq. (17). We could verify the correctness of the values obtained in this way by comparing with the results of an alternative theoretical approach [8,9,10] for calculating first-order corrections to the Gutzwiller formula in chaotic billiards, which we implemented for the three-disk system. The results turned out to be in very good agreement (on the order of 1.5 per cent, or better), with one notable exception, namely the '1' orbit, for which a distinct discrepancy (on the order of 20 per cent) persisted. We have discussed possible origins of the discrepancy although an ultimate reason could not

Table 2. Zeroth (k_0) and first (k_1) -order approximations to the complex eigenvalues of the resonances of the three-disk system with disk separation $d = 6$ (A_1 subspace), obtained by harmonic inversion of a signal of length $s_{\rm max} = 56$. For comparison, the exact quantum values $k_{\rm ex}$ are given (taken from Refs. [21,26,27]). Only resonances of the four leading bands with $\mathrm{Im}\,k \geq -0.5$ are included.

$\mathrm{Re}\,k_0$	$\mathrm{Im}\,k_0$	$\mathrm{Re}\,k_1$	$\mathrm{Im}\,k_1$	$\mathrm{Re}\,k_{\rm ex}$	$\mathrm{Im}\,k_{\rm ex}$
0.75831	-0.12282	0.61295	-0.14993	0.69800	-0.07501
2.27428	-0.13306	2.22417	-0.13960	2.23960	-0.11877
3.78788	-0.15413	3.75695	-0.15903	3.76269	-0.14755
5.29607	-0.18679	5.27282	-0.19113	5.27567	-0.18322
6.79364	-0.22992	6.77417	-0.23345	6.77607	-0.22751
7.22422	-0.49541	7.21231	-0.48189	7.21527	-0.48562
8.27639	-0.27708	8.25953	-0.27932	8.26114	-0.27491
8.77919	-0.43027	8.76958	-0.42179	8.77247	-0.42410
9.74763	-0.32082	9.73320	-0.32201	9.73451	-0.31881
10.34423	-0.37820	10.33588	-0.37289	10.33819	-0.37371
⋮	⋮	⋮	⋮	⋮	⋮
150.09512	-0.23623	150.09449	-0.23613	150.09450	-0.23613
150.76086	-0.40911	150.76004	-0.40908	150.76004	-0.40906
151.09908	-0.22292	151.09826	-0.22298	151.09826	-0.22297
151.64342	-0.22327	151.64279	-0.22321	151.64279	-0.22320
152.24814	-0.38924	152.24733	-0.38920	152.24733	-0.38919
152.60380	-0.24729	152.60298	-0.24735	152.60298	-0.24733
153.19200	-0.21587	153.19138	-0.21583	153.19138	-0.21582
153.73475	-0.36935	153.73395	-0.36932	153.73395	-0.36931
154.11072	-0.27186	154.10992	-0.27192	154.10992	-0.27190
154.74201	-0.21392	154.74140	-0.21390	154.74140	-0.21389

Table 3. Zeroth and first-order approximations to the complex eigenvalues of the resonances of the three-disk system with disk separation $d = 2.5$ (A_1 subspace), obtained from a signal of length $s_{\rm max} = 12$. The notations are the same as in Table 2. The table contains the resonances in the region $1 \leq \mathrm{Re}\,k \leq 90$ and $-0.82 \leq \mathrm{Im}\,k \leq 0$.

$\mathrm{Re}\,k_0$	$\mathrm{Im}\,k_0$	$\mathrm{Re}\,k_1$	$\mathrm{Im}\,k_1$	$\mathrm{Re}\,k_{\rm ex}$	$\mathrm{Im}\,k_{\rm ex}$
4.58118	-0.08999	4.35123	-0.05580	4.46928	-0.00157
7.14428	-0.81079	6.90301	-0.66547	7.09171	-0.72079
13.00009	-0.65163	12.93645	-0.63795	12.95032	-0.62824
17.57004	-0.68486	17.45278	-0.65154	17.50423	-0.63526
18.92585	-0.78389	18.93139	-0.72879	18.92545	-0.76629
27.88820	-0.54319	27.86253	-0.55690	27.85779	-0.54993
30.38846	-0.11345	30.34790	-0.11469	30.35289	-0.10567
32.09670	-0.62237	32.05975	-0.61112	32.06937	-0.60774
36.50664	-0.38464	36.48222	-0.38774	36.48228	-0.38392
39.81392	-0.35801	39.78247	-0.35590	39.78597	-0.35087
⋮	⋮	⋮	⋮	⋮	⋮
65.68047	-0.27378	65.66353	-0.27480	65.66387	-0.27258
67.86889	-0.28815	67.85047	-0.28896	67.85151	-0.28656
69.34446	-0.31247	69.33251	-0.30929	69.33346	-0.30925
71.08294	-0.53828	71.06684	-0.53676	71.06727	-0.53534
74.85524	-0.30224	74.83975	-0.30093	74.84053	-0.29941
77.31939	-0.31303	77.30827	-0.31116	77.30881	-0.31071
80.41789	-0.36657	80.39883	-0.36525	80.40022	-0.36289
81.69995	-0.56162	81.68874	-0.55515	81.69091	-0.55547
83.87557	-0.50399	83.86231	-0.50159	83.86311	-0.50054
85.80058	-0.41490	85.79208	-0.41566	85.79189	-0.41529

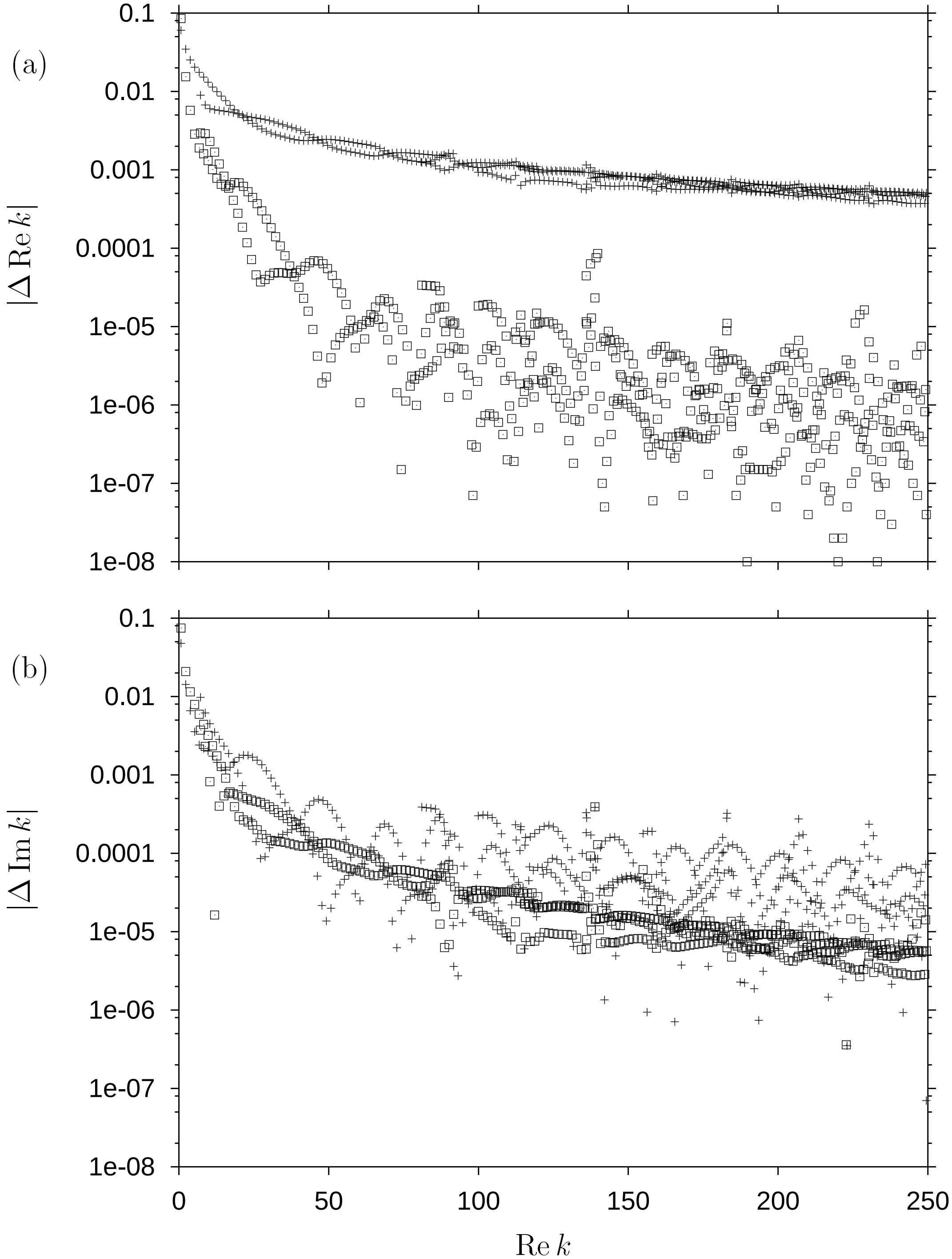

Fig. 5. The semiclassical errors of the zeroth (+) and first (⊡) -order approximations to the complex eigenvalues of the resonances of the three-disk system with $d = 6$, plotted as a function of the real part of the resonances. Only resonances with imaginary parts $\mathrm{Im}\,k \geq -0.5$ are included.

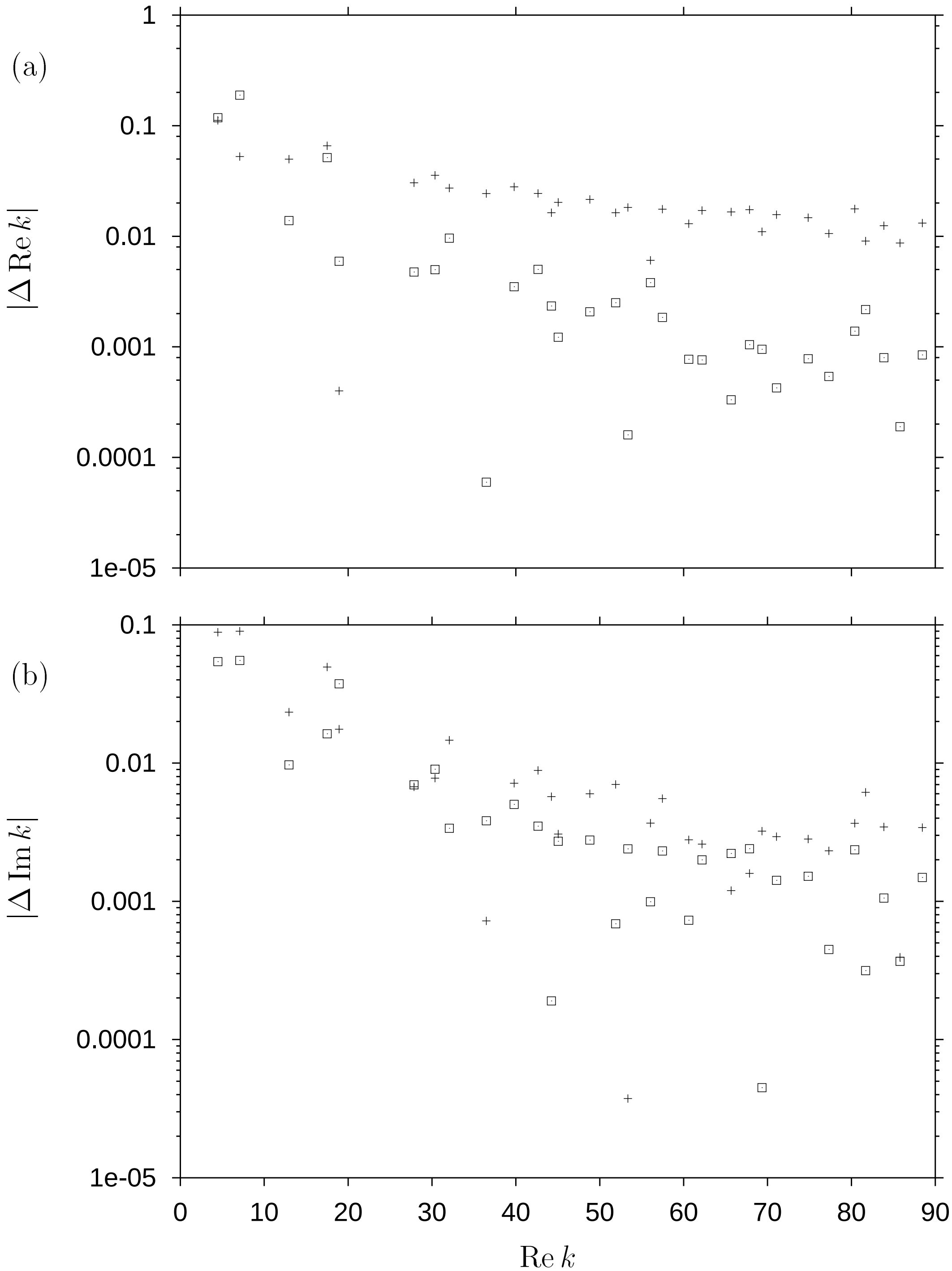

Fig. 6. As Fig. 5, but for disk separation $d = 2.5$. Only resonances with imaginary parts $\mathrm{Im}\,k \geq -0.82$ are included.

be identified. Therefore, in spite of the very good agreement of the results in all other cases, we have to conclude that the theory of $\hbar$ corrections to the Gutzwiller formula still contains unanswered questions. [We note that in fact for *integrable* systems there does not yet exist a general theory for higher-order $\hbar$ corrections to the Berry-Tabor formula at all.]

In the direct calculation of higher-order corrections to semiclassical eigenvalues from classical periodic orbit data, we first evaluated the first-order correction amplitudes to the Gutzwiller formula as given by the theory of Vattay and Rosenqvist, and then, by harmonic inversion of Eq. (24), determined the first-order $\hbar$ corrections to the semiclassical (complex) eigenvalues of resonances of the three-disk scattering system with disk separations $d = 6$ and $d = 2.5$. For

both distances, the semiclassical error, as compared to the exact quantum values, of the zeroth-order results (obtained from the Gutzwiller formula by harmonic inversion) for the real parts of the resonances could be significantly reduced by including the first-order $\hbar$ corrections: the accuracy was increased by two to five orders of magnitude for $d = 6$, and still by one to two orders of magnitude for $d = 2.5$. Only for the "most quantum" resonances, with very small real parts, the increase in accuracy was found to be rather modest. It turned out that the accuracy of the imaginary parts of the semiclassical eigenvalues of resonances was less significantly increased by the first-order corrections; here, second-order corrections would have to be considered.

Although in our calculations we have used literature values for the semiclassical resonances and for the zeroth and first-order amplitudes, we could have performed, in principle, all calculations knowing the exact quantum resonances only. The analysis of the exact quantum spectrum yields the semiclassical amplitudes, which in turn can be used to calculate the semiclassical resonances. Then, by an analysis of the difference spectrum between semiclassical and exact resonances, the first order amplitudes can be determined, which again can be used to obtain the first-order corrections to the resonances. Although we have concentrated in our examples on obtaining first-order $\hbar$ corrections, it is evident from our discussion that the next-order corrections could be obtained iteratively in an analogous manner by repeated application of Eqs. (17), and (23), (24), respectively.

In summary, we have demonstrated that harmonic inversion – as a means for circumventing the convergence problems of semiclassical trace formulae – is indeed a very efficient and universal tool, not only for semiclassical quantization, but also for the explicit calculation of higher-order $\hbar$ corrections to the semiclassical eigenvalues or resonances even in chaotic systems. Moreover, harmonic inversion does not rely on specific assumptions for the systems under consideration, and therefore an application of the methods presented in this paper to other chaotic systems will be promising and worthwhile.

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